Modeling the Growth of Thin Films in Complex 3D Geometrical Structures

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The manufacture of many advanced-material devices requires processing steps that involve the deposition or removal of thin films of materials in complex three-dimensional structures. The semiconductor industry needs modeling and simulation tools that have a predictive ability to design computer and memory circuit elements, as also the ability to predict the performance of these devices. Research at Los Alamos has been directed to this goal as a part of Cooperative Research and Development Agreements (CRADA) between the Department of Energy and the Semiconductor Research Corporation, Motorola, and Intel. More recently, similar modeling and simulation requirements have been identified for the design of microelectromechanical systems (MEMS) at Sandia National Laboratory.

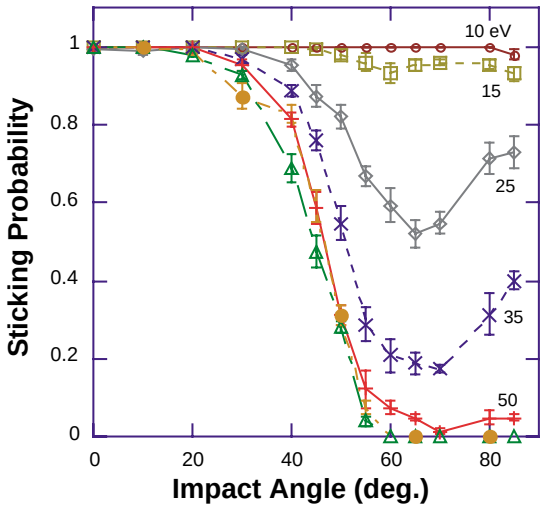

Figure 1a.

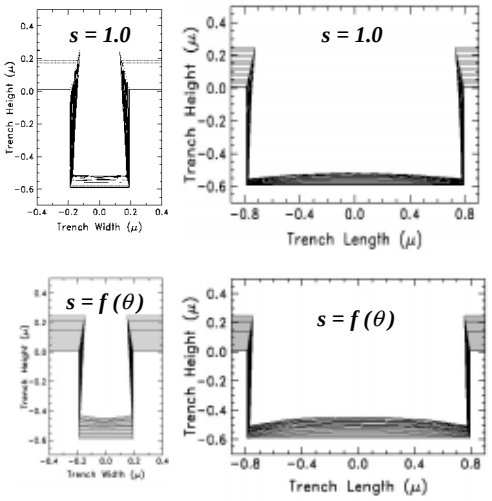

Figure 1b.

We have recently developed a computer simulation model, TopoSim-3D, for the thin-film deposition/etch processes most commonly used by the semiconductor industry. This software describes the complex three-dimensional geometric structure of the materials involved using the Los Alamos Grid Toolbox (LaGriT), which uses an unstructured grid methodology that can accurately fit any 3D geometric shape. LaGriT also treats multiple materials and the interfaces between them, and allows users to refine, de-refine, and adapt the grid as needed to optimize the mathematical treatment of the simulated process physics and chemistry. Common processes used to form thin films involve chemical or physical vapor deposition, in which material in the vapor phase is transported at low pressures to the substrate surface. TopoSim-3D models the transport process, and uses the CHEMKIN and SURFACE CHEMKIN software libraries, developed at Sandia National Laboratory, to describe the gas phase kinetics and the surface phase chemistry that occurs at the vapor/material interface. The result of modeling this transport and chemistry is a prediction of the temporal movement of the material interfaces. The nodes of the geometry grid are then moved using a finite-element algorithm, and LaGriT commands are used to further adjust node positions without damaging the shape of the material interfaces.

For many systems involving the physical vapor deposition of metals onto metal or silicon substrates, the fundamental simulation data required by TopoSim-3D is the energy-dependent probability of vapor phase material sticking to the solid surface after colliding at an angle with the surface. An example of this sticking

probability, generated using large-scale atomistic simulations of these collision processes, is shown in Figure 1a. These atomistic simulations are typically carried out on length scales of nanometers and time scales of picoseconds. By using tools such as TopoSim-3D, we are able to capture the results of these atomistic simulations for processes that involve feature length scales thousands of times larger, on time scales that are six to ten orders of magnitude longer.

On an integrated circuit chip, long rectangular channels (called trenches) are etched into an insulating material (typically silicon dioxide) and then filled with metals such as aluminum or copper. These metal lines are the structures used to connect up to millions of transistors together. It is important that these trenches be filled uniformly, avoiding any breaks in the electrical continuity between circuit elements. Figure 1b illustrates predictions by TopoSim-3D of the deposition thickness on the walls of a trench relative to the amount deposited on the floor. In the top panels of Figure 1b, the sticking probability s is approximated as a constant (unity), and in the bottom panels, the results of the atomistic simulations with angle-dependent sticking probabilities ($s = f(\theta)$) are used (at an energy of 50 eV). This atomistic data predicts that at similar deposition times, much more material will be deposited on the trench floor, and less on the trench walls.

A second example calculation using TopoSim-3D is shown in Figure 2, where we show a cutaway view of the deposition of material into an "overhang" geometry: a rectangular void partially masked by an overlaid non-adhesive material. Only the material interface is shown (although the entire 3D geometry is modeled). The color of the interface is used to display the relative local deposition rate of material– blue for the slowest growing regions, green and yellow for intermediate growth rates, and red for the fastest growing regions. For reference, the figure also shows a ghost image of the original interface at time t = 0. Geometries such as that shown here are very useful structures, because the relative deposition on the floor, walls, and roof of the overhang is a sensitive measure of the sticking probability of the depositing material. The ability of modeling and simulation tools to correctly predict the deposition profiles in such structures is essential to validating the reliability of predictions. Deposition characteristics of these structures are also a valuable aid to understanding more complicated chemical processes used by semiconductor companies.

Another example calculation (see Figure 3) shows the effect of varying the sticking coefficient on the deposition profile in a damascene structure, which consists of a trench with a cylindrical hole (via) at one end. Such structures are used as interconnects in newly proposed technologies that use copper as a conducting metal. As in Figure 2, the interface colors reveal the relative growth rates of the different regions of the interface. Note that the material deposition uniformity is much better when the deposition material sticking probability is low. In such cases, the material being deposited bounces around the interior of the structure many times before it sticks, thereby allowing more material to reach the more remote, indirectly accessible regions of the structure. Simulations such as this suggest that chemical deposition processes characterized by low sticking probabilities of the reactive species may be superior to physical deposition processes that typically have much higher sticking probabilities.

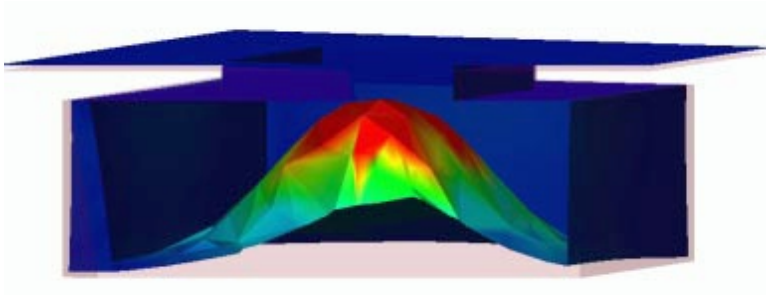

Figure 2.

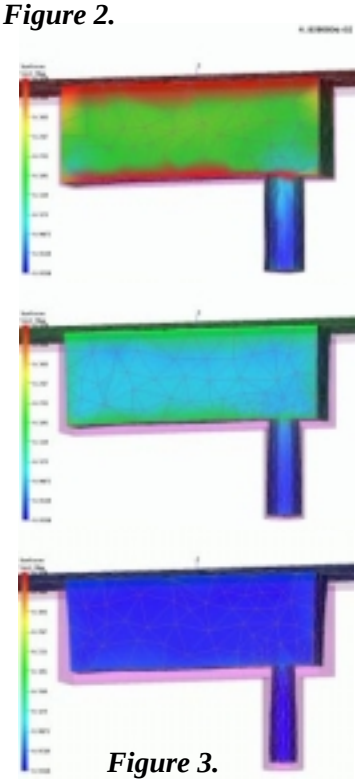

Figure 3.